

## Application of the Harris-Nesbet Method to a Dipole Coupling Potential\*

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Elastic and inelastic cross sections for a two-channel model problem, in which dipole coupling is assumed, are calculated in the Harris-Nesbet method and compared with direct solutions of the Schroedinger equation. Two different coupling potentials are considered, one of which permits exact solution in terms of known functions, while the other requires a numerical solution. Results accurate to 1% are obtained for a non-degenerate case when a minimum representation for the wavefunction is taken as a combination of Slater orbitals and spherical Bessel and Neumann functions. For a degenerate case, it is found to be necessary to use sinusoidal energy-dependent terms in addition to Slater orbitals for a description of the internal part of the wave function and that, for the external part, only the leading asymptotic term of the spherical Bessel and Neumann functions need be retained.

### I. INTRODUCTION

Cross sections for a two-channel model problem, in which the off-diagonal potential is taken to be a dipole, are calculated by the Harris-Nesbet variational method and compared with those obtained by solving the differential equations.

Harris [1] has proposed an algebraic expansion technique for the solution of the differential equation which arises for elastic scattering processes. The method was restricted in that the phase shifts could be calculated only at certain energies—the Harris eigenvalues of the problem. However, this restriction has been removed by Nesbet [2], who extended the Harris technique so that phase shifts would be calculated at arbitrary energies. Nesbet [3] further developed a formalism which included inelastic processes—referred to here as the Harris-Nesbet method—and

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successfully applied it to a two-channel model problem in which the off-diagonal coupling between the two channels is taken to be a constant step potential. An attractive feature of the Harris–Nesbet method is that it is essentially algebraic in nature.

Seiler [4] has applied the Harris–Nesbet method to the scattering of positrons and electrons from atomic hydrogen in the  $1s$ - $2s$ - $2p$  close-coupling approximation. His results agree well with calculations [5–7] in which the closely coupled equations are solved numerically for energies  $E < 0.75$  Ry, where only elastic scattering is energetically possible. However, for  $E > 0.75$  Ry., where the  $1s$ ,  $2s$ , and  $2p$  hydrogenic states are energetically accessible, he was unable to obtain satisfactory results when only Slater basis functions and spherical Bessel and Neumann functions were used in the expansion of the wave functions. The source of the difficulty is the coupling of the degenerate  $2s$  and  $2p$  states of atomic hydrogen, which gives rise to a long-range off-diagonal dipole. Seiler, Oberoi and Callaway [8] added energy-dependent sinusoidal terms to the basis set employed by Seiler [4] and used this set to obtain  $S$ -wave partial cross sections for scattering of electrons by atomic hydrogen in the three-state approximation for  $E > 0.75$  Ry. Their results agree to within 1.0% with numerical calculations of Burke *et al.* [7].

We investigate two-channel model problems, both degenerate and nondegenerate, each having an off-diagonal dipole potential. The models are discussed in Section II together with the relevant equations of the Harris–Nesbet method. Further, the asymptotic equations for the degenerate model problem are solved analytically in Section IIA where it is found to be necessary to include, in the expansion of the wave functions, other terms in addition to those retained by Seiler [4]. In Section III we discuss alternative methods of including these additional terms in the degenerate dipole coupling case, and further we show that such terms are not required in the nondegenerate case.

## II. THE HARRIS–NESBET METHOD FOR A DIPOLE COUPLING POTENTIAL

The radial equation for an  $N$ -channel system may be written

$$\sum_j (H_{ij} - E \delta_{ij}) \psi_j^\nu = 0, \quad (1)$$

where  $i$  and  $j$  range over the open channels,  $H_{ij}$  are the matrix elements of the Hamiltonian operator, and  $E$  is the total energy of the system. The Harris–Nesbet method assumes that the radial function for channel  $j$ , when the system is initially in channel  $\nu$ , may be given by

$$\psi_j^\nu(r) = \Phi_j^\nu(r) + \alpha_{0j}^\nu S_j(r) + \alpha_{1j}^\nu C_j(r), \quad (2)$$

where  $\Phi_j^\nu(r)$  represents the internal part of the wavefunction which may be expanded in normalized functions.

Further, the functions  $S_j$  and  $C_j$  of Eq. (2) are required to satisfy the boundary conditions

$$\begin{aligned} S_j(r) &\underset{r \rightarrow \infty}{\sim} \sin(k_j r - l_j \pi/2), \\ C_j(r) &\underset{r \rightarrow \infty}{\sim} \cos(k_j r - l_j \pi/2). \end{aligned} \quad (3)$$

An appropriate variational formalism is then applied to find the arbitrary parameters. Details of the method are contained in Nesbet [3]. For example, on applying the Kohn variational method, elements of the reactance  $R$ -matrix can be related to the  $\alpha$ -coefficients by

$$\alpha_{0j}^\nu = \delta_{\nu j}; \quad \alpha_{1j}^\nu = (k_\nu/k_j)^{1/2} R_{\nu j}. \quad (4)$$

Partial cross sections for a transition  $\nu \rightarrow j$  are related to the  $R$ -matrix elements through

$$Q_{\nu j} = 4\pi |[R/(1 - iR)]_{\nu j}|^2/k_\nu^2 \quad (5)$$

We are required to choose functions  $\Phi_j^\nu$ ,  $S_j$ , and  $C_j$  such that the interaction region is adequately spanned. Let us examine two-channel model problems which have an off-diagonal dipole potential, since this includes the dominant long-range feature which is inherent, for example, in low-energy electron-hydrogen scattering. We have studied two such models, each having the same diagonal elements. The Hamiltonian operator is (in Rydberg units)

$$\begin{aligned} H_{11} &= -[d^2/dr^2 - l_1(l_1 + 1)/r^2], \\ H_{22} &= -[d^2/dr^2 - l_2(l_2 + 1)/r^2] + \Delta E. \end{aligned}$$

The off-diagonal elements are

*Case I.*

$$\begin{aligned} H_{12} &= H_{21} = b/r^2 & (r > r_0), \\ H_{12} &= H_{21} = 0 & (r < r_0). \end{aligned} \quad (6a)$$

*Case II*

$$H_{12} = H_{21} = b(1 - e^{-r})^3/r^2, \quad (6b)$$

where  $l_j$  and  $k_j$  are the orbital angular momentum and wavenumber of the scattered particle in channel  $j$ , respectively;  $b$  is the coupling parameter; and  $\Delta E$  is the energy separation of the channels given by

$$\Delta E = (k_1^2 - k_2^2). \quad (7)$$

The solution for the wavefunction in Case I can be expressed in terms of known functions (if  $\Delta E = 0$ ). The elements of the  $R$  matrix are determined by matching functions and derivatives at the potential discontinuity  $r = r_0$ . Numerical integration must be employed in Case II.

## IIA: DEGENERATE ASYMPTOTIC SOLUTIONS

We consider the solution of the asymptotic equations in the degenerate case, in which both channels have the same energy  $k^2$ . The coupled differential equations for large  $r$  are

$$\sum_i \left[ \left( \frac{d^2}{dr^2} + k^2 \right) \delta_{ij} - \frac{M_{ij}}{r^2} \right] \psi_j(r) = 0; \quad i, j = 1, 2 \quad (8)$$

where the matrix  $M$  is given by

$$M_{ij} = l_i(l_i + 1) \delta_{ij} + a_{ij}$$

with

$$a_{ij} = \begin{cases} 0 & i = j \\ b & i \neq j \end{cases} \quad (9)$$

A general solution of Eq. (8) is [9]

$$\psi_j(r) = \sum_i A_{ji} \Phi_i(r), \quad (10)$$

where  $A$  is a real, orthogonal matrix which diagonalizes  $M$  so that

$$A_n(\Lambda_n + 1) \delta_{nm} = \sum_{ij} A_{ni}^{-1} M_{ij} A_{jm}. \quad (11)$$

The functions  $\Phi_i$  can be written in terms of the Bessel functions of order  $\Lambda_n + \frac{1}{2}$  and  $-\Lambda_n - \frac{1}{2}$ .

Consider the case when  $l_1 = 0$  and  $l_2 = 1$  so that the  $M$  and  $A$  matrices can be written as

$$M = \begin{pmatrix} 0 & b \\ b & 2 \end{pmatrix}; \quad A = \begin{pmatrix} b & b \\ \lambda_1 & \lambda_2 \end{pmatrix}$$

where  $\lambda_{1,2} = 1 \pm \sqrt{1 + b^2}$ .

In order to use the Harris–Nesbet method we are required to construct solutions which have the asymptotic form (from Eqs. (2) and (4)):

$$\psi_j^\nu(x) \underset{x \rightarrow \infty}{\sim} k^{-1/2} [\sin(x - l_j \pi/2) \delta_{j\nu} + \cos(x - l_j \pi/2) R_{j\nu}] \quad (12)$$

For Eqs. (8), we may choose to write solutions in the form [with  $\Phi_j^\nu = 0$ ]

$$\psi_j^\nu(x) = k^{-1/2} [S_j(x) \delta_{j\nu} + C_j(x) R_{j\nu}] \quad j = 1, 2. \quad (13)$$

Equating (10) and (13) we obtain

$$\begin{aligned} S_1(x) &= \sin x + A(\alpha R_{11}) \sin x + B(\alpha \det R) \cos x, \\ C_1(x) &= \cos x - B(\alpha) \sin x + A(-\alpha R_{22}) \cos x, \\ S_2(x) &= -\cos x + x^{-1} \sin x + C(\alpha \det R) \sin x - A(-\alpha R_{22}) \cos x, \\ C_2(x) &= \sin x + x^{-1} \cos x + A(\alpha R_{11}) \sin x + C(\alpha) \cos x, \end{aligned} \quad (14)$$

where

$$\begin{aligned} \alpha &= b/R_{12}, \\ \det R &= R_{11}R_{22} - R_{12}R_{21}, \\ A(\beta) &= -\frac{\beta}{2x} - \frac{b^2}{8x^2} + \frac{\beta b^2}{48x^3} - \dots, \\ B(\beta) &= -\frac{\beta}{2x} + (6 + \beta) \frac{b^2}{48x^3} - \dots, \\ C(\beta) &= \frac{\beta}{2x} + (4 - \beta) \frac{b^2}{48x^3} - \dots. \end{aligned} \quad (15)$$

We note that each term of the functions  $A$ ,  $B$ , and  $C$  depends on the coupling strength  $b$ . When there is no coupling between the channels, the expansions for the asymptotic terms, Eq. (14), reduce to spherical Bessel and Neumann functions. However, when coupling is present in this degenerate case, terms of order  $O(x^{-1})$  are introduced, which are of the same order as those included in the zero-coupling case, and solutions of the asymptotic Eqs. (8) are no longer pure spherical Bessel and Neumann functions. Thus, in the degenerate dipole case, in order to span properly the interaction region, at least the first term in the functions  $A$ ,  $B$ , and  $C$  must be included in expansions (2).

## III. COMPUTATIONAL PROCEDURES

## A. Exact Solution

## Case I

Solution for this potential [see Eq. (6a)] can be expressed in terms of Bessel functions provided  $\Delta E = 0$ . We consider specifically  $b = -6$ ,  $l_1 = 0$  and  $l_2 = 1$ , which corresponds to a typical value for atomic hydrogen. For  $r < r_0$  two linearly independent solutions of (8) which are regular at the origin are

$$\begin{aligned}\psi_1^1 &= \text{Pr } j_0(kr), & \psi_2^1 &= 0 \\ \psi_1^2 &= 0, & \psi_2^2 &= Qr j_1(kr)\end{aligned}\quad (16)$$

For  $r > r_0$ , the solutions can be expressed in terms of function  $f_{\mu_n}^{\pm}(r) = r^{1/2} J_{\pm\mu_n}(r)$ , in which

$$\mu_1 = [\frac{5}{4} + \sqrt{37}]^{1/2}, \quad \mu_2 = i[\sqrt{37} - \frac{5}{4}]^{1/2}, \quad (17)$$

and  $J_{\mu}(kr)$  is a Bessel function [9]. The components of the total wavefunction are expressed in a form similar to (10):

$$\psi_j^{\nu}(kr) = \sum_i A_{ji} \chi_i^{\nu}(kr), \quad (18)$$

in which

$$\begin{aligned}\chi_1^{\nu} &= C_{\mu_1}^+ f_{\mu_1}^+ + C_{\mu_1}^- f_{\mu_2}^-, \\ \chi_2^{\nu} &= C_{\mu_2}^+ f_{\mu_2}^+ + C_{\mu_2}^- f_{\mu_2}^-.\end{aligned}\quad (19)$$

The asymptotic form of the functions  $f_{\mu}$  is

$$f_{\mu} \sim \left(\frac{2}{\pi k}\right)^{1/2} \cos \left[ kr - \left(\frac{\mu}{2} + \frac{1}{4}\right) \pi \right]. \quad (20)$$

The constants  $C_{\mu}^{\pm}$  above can be related to the as yet unknown elements of the  $R$  matrix by requiring that Eqs. (12) and (19) must be equivalent asymptotically. Analytic expressions for the  $R$  matrix are finally obtained by matching the interior and exterior solutions (functions and derivatives) at  $r = r_0$ . Since the resulting expressions for the  $R$  matrix elements are quite complicated, we will not reproduce them here.

## Case II

In this case, since analytic solutions are not known, it is necessary to solve Eq. (1) numerically. Further, the unphysical discontinuity in the elements of the Hamil-

tonian of Case I is not present. We solve (1) for both a degenerate and a non-degenerate two channel problem, using the same values of the parameters  $b$ ,  $l_1$ ,  $l_2$  as in Case I above. Numerical solutions are obtained by integrating the equations outwards and inwards by Numerov's method, with subsequent matching to obtain a final continuous solution. The asymptotic expansion method of Burke and Schey [5] is used to determine the  $R$ -matrix from the function  $\psi_j^p(r)$ . A combination of these methods has been outlined by Smith et al. [10]. The  $R$ -matrices and cross sections are found to be independent of the integration parameters to at least 4 significant figures. The numerical solutions are used as a standard against which results from the Harris-Nesbet method for various choices of functions  $\Phi$ ,  $S$ , and  $C$  are judged.

### B. The Harris-Nesbet Method

We will now describe the companion calculation by the Harris-Nesbet method.

We choose the internal part of wave function (2) to be represented by Slater orbitals:

$$\Phi_j^p(r) = \sum_{a=1}^{n_j} c_{jv,a} \eta_{ja}(r), \quad (21)$$

with

$$\eta_{ja}(r) = N_{ja} r^{l_j+1} e^{-\zeta_{ja} r}, \quad (22a)$$

where the  $c_{jv,a}$  are variationally determined parameters,  $N_{ja}$  are normalization constants for the Slater orbitals, and the exponents  $\zeta_{ja}$  are selected to span adequately the short-range portion of the interaction region. These exponents are chosen such that the maxima of the Slater terms occur at various spatial positions in the interaction region. The maximum of a Slater orbital occurs at  $r_M = (l_j + 1)/\zeta_{ja}$ . Hence, by choosing a set of  $r$  values in the interaction region, a set of corresponding  $\zeta_{ja}$  coefficients is simply obtained. However, if the set of  $r$  values is too dense, numerical difficulties will occur in solving the required eigenvalue equation, since some of the functions become linearly dependent.

In those problems involving degenerate channels, we may supplement the basis function described above by normalized functions of the form

$$\eta_{js}^{(m)}(r) = N_{js} \frac{(1 - e^{-\beta r})^{l_j+m+2}}{r^m} \begin{cases} \sin k_j r & s = 1, \\ \cos k_j r & s = 2, \end{cases} \quad (22b)$$

where  $N_{js}$  are normalization constants and the exponent  $m$  takes on values 1 or 2. This choice is made since Eq. (14) indicates that terms of the form (22b) are important in the exact solutions of Eqs. (8).

We choose spherical Bessel and Neumann functions to represent the  $S_j$  and  $C_j$  functions. To ensure that they behave properly for small values of  $r$ , we multiply by cut-off factors of the form  $(1 - e^{-\beta r})^n$ . Parameter  $n$  is chosen so that the functions decrease at least as fast as  $r^{l_j+1}$  for small  $r$ . Values of the cross sections are insensitive to  $\beta$  for  $\beta \simeq 1$ .

To determine if the above minimum choices for  $\Phi_j^v$ ,  $S_j$ , and  $C_j$  are sufficient to guarantee calculated cross sections accurate to 1% in the Harris-Nesbet method, we now consider first a nondegenerate case and then a degenerate case.

1. *Non-Degenerate Situation.* For this case we choose, in Eq. (6),  $\Delta E = 0.75$  Ry, which is the splitting of the  $n = 1$  and  $n = 2$  levels in atomic hydrogen. Only the "smooth" Hamiltonian of Case II is considered. We cannot decouple the equations in the manner employed for the asymptotic Eqs. (8), but examination of an asymptotic expansion of the solutions shows that the lowest order correction terms due to a nondegenerate dipole coupling potential, are  $O(x^{-2})$ . Thus, we may expect that pure spherical Bessel and Neumann functions together with Slater orbitals may be sufficient for the case  $l_1 = 0$  and  $l_2 = 1$ .

As noted by Harris and Michels [11] for a two-channel Huck problem more rapid convergence is achieved for the cross sections than for the individual elements of the  $R$ -matrix. We find this to be true for our model problems also and thus we will give values of the partial cross sections rather than the individual  $R$ -matrix elements.

Table I gives partial cross sections for an energy  $E = 1.0$  Ry. Column A lists

TABLE I  
Partial-wave cross sections  $Q_{ij}$  for a nondegenerate Case II with  
 $E = 1.0$  Ry,  $\Delta E = 0.75$  Ry,  $l_1 = 0$ ,  $l_2 = 1$ , and  $b = -6^a$

	A	B	C
$Q_{11}$	7.445	7.390	7.391
$Q_{12}$	0.1780	0.1786	0.1779
$Q_{22}$	14.53	14.52	14.47

<sup>a</sup> Column A: numerical; Column B: Kohn variational method; Column C: Rubinow variational method.

the values obtained from a numerical solution. Results obtained in the Harris-Nesbet method with the Kohn and Rubinow variational methods are given in Columns B and C. Twenty Slater orbitals are included in the internal function  $\Phi_j^v$  for each channel, and spherical Bessel and Neumann functions are used for the  $S_j$  and  $C_j$  functions. Nesbet [3] has suggested a criterion, related to a ratio of certain



matrix elements, for choosing which variational method is superior for a given energy. For Table I this criterion suggests that the Rubinow method (Column C) gives superior results to those calculated by the Kohn method. We note that with either method the agreement with numerical calculations is within 0.8% and that the variational results agree to within 0.4%. This holds true for the range of energies  $0.8 \leq E \leq 2.0$  Ry. investigated, with  $\Delta E = 0.75$  Ry.

2. *Degenerate Situation.* For this case we have  $\Delta E = 0$  in Eq. (6). In Section IIA we find that pure spherical Bessel and Neumann functions are not the correct solutions to the asymptotic equations, so we expect that the minimum choices for  $\Phi_j^v$ ,  $S_j$ , and  $C_j$  will not be sufficient for this degenerate case.

### Case I

Partial cross sections for the sharply cutoff potential of Case I are given in Table II. The exact results (A) are compared with those obtained from the Kohn (B) and Rubinow (C) procedures for two different values of the wave vector  $k$ . The basis set included 13 Slater orbitals and six trigonometric functions in each channel.

TABLE II

Partial cross sections  $Q_{ij}$  for the degenerate problem. Case I: sharply cutoff potential<sup>a</sup>

	$k = 0.3$		
	A	B	C
$Q_{11}$	18.717	18.710	18.710
$Q_{12}$	8.489	8.547	8.547
$Q_{22}$	15.198	15.105	15.105
	$k = 0.9$		
	A	B	C
$Q_{11}$	1.101	1.116	1.115
$Q_{12}$	0.141	0.147	0.147
$Q_{22}$	3.644	3.622	3.623

<sup>a</sup> The fixed parameters are  $l_1 = 0$ ,  $l_2 = 1$ ,  $b = -6$ ,  $r_0 = 1$ . Columns as in Table I.

The variational calculation for this potential has certain special features. For  $r < r_0$ , the wave functions in the interior region are pure spherical functions, and the Slater orbitals are actually not needed. The discontinuous nature of the coupling term produces a discontinuous second derivative of the wavefunction. For this reason, the convergence of the variational results is not rapid. However, it is seen

that results of acceptable quality, i.e., discrepancies of only a few percent between exact and variational results are obtained. All integrals appearing in the variational calculation are calculated analytically.

### Case II

Here we have a smooth coupling potential. We have investigated two methods by which additional terms may be incorporated in an expansion of wave functions  $\psi_j^v$ .

We choose fifteen Slater orbitals to represent the internal functions  $\Phi_j^v$  for each channel, and augment our minimum representation for  $S_j$  and  $C_j$  functions by choosing them to be given by Eq. (14). Since these terms depend explicitly on the  $R$ -matrix which we are trying to calculate, we obtain initial estimates for  $R_{ij}$  by using spherical Bessel and Neumann functions for  $S_j$  and  $C_j$ , respectively. With this estimate, we iterate Eq. (14) until convergence of the partial cross sections is obtained.

Table III gives partial cross sections for an energy  $E = 0.25$  Ry. Column A

TABLE III  
Partial-wave cross sections  $Q_{ij}$  for degenerate Case II with  
 $E = 0.25$  Ry,  $l_1 = 0$ ,  $l_2 = 1$ , and  $b = -6^a$

		A	B	C	D	E	F	G
$Q_{11}$	(a)	3.653	10.700	3.165	3.665	3.650	3.650	3.652
	(b)		3.260	5.451	3.717	3.650	3.650	3.652
$Q_{12}$	(a)	0.0094	0.0021	0.0117	0.0094	0.0094	0.0094	0.0095
	(b)		0.0010	0.0070	0.0092	0.0094	0.0094	0.0095
$Q_{22}$	(a)	45.515	46.032	45.482	45.538	45.536	45.537	45.516
	(b)		40.349	45.526	45.538	45.536	45.537	45.516

<sup>a</sup> See text for a description of rows and columns.

lists the values obtained from a numerical solution while Columns B-F give results obtained in the Harris-Nesbet method, when terms up to  $O(x^{-1})$  are included in the functions  $S_j$  and  $C_j$ . Inclusion of only spherical Bessel and Neumann functions in Eq. (14) leads to the cross sections given in Column B, which are in poor agreement with those given in Column A. Successive iterations are listed in Columns C, D, and E. The values in Column F are a result of the use of the numerical  $R$ -matrix elements in Eq. (14). An examination of Columns E and F shows that when one term is taken in functions A, B, and C of Eq. (15), iterations on the  $R$ -matrix elements have converged satisfactorily. Finally, Column G

is obtained when we include terms up to  $O(x^{-2})$  in Eqs. (14) and (15) and the numerical  $R$ -matrix elements are used in computing the functions  $A$ ,  $B$ , and  $C$  of Eq. (15). Thus we conclude that only the first term need be retained for this case of  $l_1 = 0$  and  $l_2 = 1$ . This holds true for the range of energies  $0.01 \leq E \leq 1.0$  Ry investigated.

The partial cross sections referred to in rows (a) of Table III are calculated using the Kohn variational method and those in rows (b), the Rubinow. According to the Nesbet criterion [3], cross sections in rows (a) are superior to those in rows (b). However, we find that the two methods predict the same results for the degenerate cases studied.

An alternative method for incorporating additional terms in an expansion of  $\psi_j^v$  is to use spherical Bessel and Neumann functions for  $S_j$  and  $C_j$  and to augment our minimum representation for the internal function  $\Phi_j^v$ . To the basis set which previously consisted of Slater orbitals we add sinusoidal energy-dependent functions presented in Eq. (22b). These basis functions should provide the corrections which are included through use of functions  $A$ ,  $B$ , and  $C$  of Eq. (15) in the first method. The advantage of the second method is that functions (22b) will be weighted by variationally derived parameters and we do not need to iterate our solution with respect to the  $R$ -matrix elements. A disadvantage, however, is that these additional basis functions are energy dependent and so an eigenvalue equation [(55) of Ref. 3] has to be solved for every energy, whereas when only Slater orbitals are included in  $\Phi_j^v$  it need only be solved once.

Table IV gives partial cross sections for an energy  $E = 0.25$  Ry. in the degenerate case with  $l_1 = 0$ ,  $l_2 = 1$ , and  $b = -6$ . Column A lists the values obtained from a numerical solution, while Columns B-D give results obtained in the Harris-Nesbet method. In Columns B and C spherical Bessel and Neumann functions,

TABLE IV  
Partial-wave cross sections  $Q_{ij}$  for degenerate Case II with  
 $E = 0.25$  Ry,  $l_1 = 0$ ,  $l_2 = 1$ , and  $b = -6^a$

		A	B	C	D
$Q_{11}$	(a)	3.653	3.646	3.676	3.676
	(b)		3.642	3.649	3.649
$Q_{12}$	(a)	0.0094	0.0101	0.0095	0.0095
	(b)		0.0073	0.0094	0.0094
$Q_{22}$	(a)	45.515	45.499	45.497	45.488
	(b)		45.540	45.513	45.513

<sup>a</sup> See text for a description of rows and columns.

which are cut-off so that they have the correct behavior for small  $r$ , are used for the  $S_j$  and  $C_j$  functions. Fourteen Slater orbitals are included in the internal functions  $\Phi_j^v$  for each channel together with sinusoidal functions (22b) with  $m = 1$  and  $m = 1$  and 2, respectively, for Columns B and C. The only difference in the choice of functions for Columns C and D is that, for Column D, we use the leading term for the  $S_j$  and  $C_j$  functions whereas, for Column C, we employ spherical Bessel and Neumann functions. The Nesbet criterion suggests that results in row (b) are superior to those in row (a).

For this degenerate case we obtain results accurate to 0.8% when we augment  $\Phi_j^v$  by incorporating energy-dependent sinusoidal terms (22b) of one order greater than the appropriate spherical Bessel and Neumann functions. Further, we find that we need only retain the leading asymptotic term in the  $S_j$  and  $C_j$  functions.

We conclude that, in problems which contain a dipole coupling potential, a minimum expansion for wave functions, in terms of Slater orbitals and spherical Bessel and Neumann functions, is sufficient when the energies of the channels are unequal but it is insufficient when they are equal. In the latter (degenerate) case, a method which can easily be extended to multichannel problems with arbitrary angular momenta is to include sinusoidal energy-dependent terms of type (22b) in addition to Slater orbitals for a description of the internal wave function and, for the external part of  $\psi_j^v$ , to retain only the leading asymptotic term in the  $S_j$  and  $C_j$  functions.

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